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The Determination of the Scattering Potential from the Spectral Measure Function
Part II: Point Eigenvalues and Proper Eigenfunctions

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Abstract

In Part I of this paper [1] we restricted ourselves to the consideration of weight operators which led to Hamiltonians H whose spectra were identical to the spectrum of a given unperturbed Hamiltonian H_o. In this part of the paper we propose to show how one may choose weight operators which lead to Hamiltonians H having spectra different from that of H_o. To make the discussion more concrete we shall take the case where H_o has a purely continuous spectrum extending from 0 to ∞ and where H has a spectrum which has a continuous part which coincides with the spectrum of H_o and, in addition, has negative point eigenvalues.

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1. Introduction

In Part I of this paper [1] we restricted ourselves to the consideration of weight operators which led to Hamiltonians H whose spectra were identical to the spectrum of a given unperturbed Hamiltonian H_o. In this part of the paper we propose to show how one may choose weight operators which lead to Hamiltonians H having spectra different from that of H_o. To make the discussion more concrete we shall take the case where H_o has a purely continuous spectrum extending from 0 to ∞ and where H has a spectrum which has a continuous part which coincides with the spectrum of H_o, and, in addition, has negative point eigenvalues. However, the procedure which is discussed is capable of being generalized considerably, at least in a formal fashion.

It is our objective to find operators U and U_o such that

$$WU^* = U_o \tag{1.1}$$

$$U_o = U^{-1} \tag{1.2}$$

where W is the weight operator. We wish H to be obtained from

$$H = UH_oU_o = UH_oU^{-1} . \tag{1.3}$$

Clearly (1.3) cannot hold if H_o and H have a different spectrum, which is the case being considered here. We shall have to define a vector space larger than Hilbert space such that the spectrum of H_o in this larger space is the same as that of H in this space.

It will be possible to carry out the extension of the Hilbert space to the larger space in terms of the Q-representation which is the representation in which K is triangular in the sense described in Part I, i.e.,

$$< q|U|q' > = \delta(q-q') + \varepsilon < q|K|q' > , \tag{1.4}$$

where

(1.5) $$< q|K|q' > = 0 \qquad \text{for } q' > q.$$

Like Part I this paper has two main divisions. In the first (Sections 2 and 3) we shall characterize the weight operator assuming the operator H and its spectrum given. In the second division (Section 5) we shall show how H can be obtained from the weight operator. We shall see that in addition to prescribing the weight operator which gives the weight function of the eigenfunction of the continuous spectrum and prescribing the boundary conditions which these eigenfunctions must satisfy, we shall have to give the normalization constants and eigenvalues of the proper eigenfunctions. Furthermore, we shall have to specify a set of 'eigenfunctions' of H_o which span the vector space which must be added to the Hilbert space to assure us that the spectrum of H_o coincides with that of H.

2. The eigenfunctions of the unperturbed Hamiltonian and the extended vector space

Since we shall work with a vector space larger than Hilbert space, it will be useful to introduce a projection operator which shall be denoted by $\eta(H_o)$. This operator is to have the property that

(2.1) $$\eta(H_o)|\emptyset > = |\emptyset >$$

if the state $|\emptyset >$ is in the Hilbert space, and that

(2.2) $$\eta(H_o)|\emptyset > = 0$$

if $|\emptyset >$ is in that part of the vector space which is orthogonal to the Hilbert space.

As in Part I we shall denote the eigenstates of H_o, A_o belonging to the eigenvalues E, a, respectively, by $|H_o,A_o;E,a >$. Since we are assuming that the spectrum of H_o is continuous and ranges from zero to $+\infty$, we shall express

the fact that the $|H_o,A_o;E,a>$ for $E > 0$ are a complete set in the Hilbert space by

$$\iint |H_o,A_o;E,a> \eta(E)dEda < H_o,A_o;E,a| = \eta(H_o), \tag{2.3}$$

$\eta(E)$ being the usual Heaviside step function.

We shall extend the definition of the operator H_o so that it has eigenvalues which correspond to the negative point eigenvalues E_i of the operator H. Toward this end we introduce 'eigenfunctions' $|H_o,A_o;E,a>$ which are defined for $E < 0$ in the vicinity ΔE_i of each eigenvalue E_i of H. These eigenfunctions are to span a vector space orthogonal to the Hilbert space. We shall characterize this extended space by working in the Q-representation. Every operator A defined in Hilbert space can be represented as an integral operator with the kernel $<q|A|q'>$. If the operator A as defined in the extended space has the same form as an integral operator in the Q-representation when operating on vectors in the extended space, we shall call the operator A 'a Q-extended operator'. We shall discuss Q-extended operators in more detail in Section 4.

In particular we shall take H_o as a Q-extended operator. Hence for $E < 0$, the eigenfunctions $|H_o,A_o;E,a>$ are defined by

$$\int_{q_o}^{q_1} <q|H_o|q'> dq' <q'|H_o,A_o;E,a> = E <q|H_o,A_o;E,a> \tag{2.4}$$

for E in the vicinity ΔE_i of each point eigenvalue E_i of H. If, for example, $H_o^Q = -\frac{d^2}{dq^2}$ (where the superscript Q means that H_o is expressed in the Q-representation) we should solve for $<q|H_o,A_o;E,a>$ from

$$-\frac{d^2}{dq^2} <q|H_o,A_o;E,a> = E <q|H_o,A_o;E,a> .$$

Not every solution of (2.4) will be used to define an eigenfunction of H_o in the extended space, for we shall require that $<q|H_o,A_o;E,a>$ be quadratically integrable functions of q in the vicinity of q_o. If $q_o = -\infty$ then a necessary

condition is

$$\lim_{q \to -\infty} \langle q|H_o,A_o;E,a\rangle = 0 . \tag{2.5}$$

As we shall see in Section 6, this condition is a necessary condition for the bound states of H to be quadratically integrable functions of q.

We shall designate the function $\langle q|H_o,A_o;E,a\rangle$ which is a solution of (2.4) subject to the above condition by the ket $|H_o,A_o;E,a\rangle$. The corresponding bra $\langle H_o,A_o;E,a|$ will be used to denote the function $\langle H_o,A_o;E,a|q\rangle$ where

$$\langle H_o,A_o;E,a|q\rangle = \langle q|H_o,A_o;E,a\rangle^* \tag{2.6}$$

where the asterisk denotes complex conjugate.

Let us denote by ${}_B\langle H_o,A_o;E,a|q\rangle^*$ another set of functions which satisfy both (2.4) and

$$\int_{q_o}^{q_1} {}_B\langle H_o,A_o;E,a|q\rangle \, dq \, \langle q|H_o,A_o;E',a'\rangle = \delta(E-E')\delta(a,a'). \tag{2.7}$$

We also require that the eigenfunctions of H_o belonging to the positive spectrum be orthogonal to the eigenfunctions of the extended space, i.e.,

$$\eta(-E)\,\eta(E')\int_{q_o}^{q_1} {}_B\langle H_o,A_o;E,a|q\rangle \, dq \, \langle q|H_o,A_o;E',a'\rangle = 0. \tag{2.7a}$$

$$\eta(-E)\,\eta(E')\int_{q_o}^{q_1} \langle H_o,A_o;E,a|q\rangle \, dq \, \langle q|H_o,A_o;E',a'\rangle = 0. \tag{2.7b}$$

We can write

$$\int_{q_o}^{q_1} \langle q|H_o|q'\rangle\langle q'|H_o,A_o;E,a\rangle_B = E\,\langle q|H_o,A_o;E,a\rangle_B \, , \tag{2.8}$$

where $\langle q|H_o,A_o;E,a\rangle_B$ is defined by

$$\langle q|H_o,A_o,E,a\rangle_B = {}_B\langle H_o,A_o;E,a|q\rangle^*. \tag{2.9}$$

The bra ${}_B\!\!< H_o,A_o;E,a|$ is used to denote ${}_B\!\!< H_o,A_o;E,a|q >$ and the ket $|H_o,A_o;E,a >_B$ is used to denote $< q|H_o,A_o;E,a >_B$. The subscript B is used to denote the fact that ${}_B\!\!< H_o,A_o;E,a|$ is the 'bi-orthogonal' bra to $|H_o,A_o;E,a >$.

If I is the identity operator of the entire vector space, we write

$$\int_{q_o}^{q_1} |q > dq < q| = I, \tag{2.10}$$

$$< q|q' > = \delta(q-q') . \tag{2.10a}$$

Then (2.7) can be written abstractly as

$$\begin{aligned} {}_B\!\!< H_o,A_o;E,a|H_o,A_o;E',a' > &= \delta(E-E')\delta(a,a'), \\ < H_o,A_o;E,a|H_o,A_o;E',a' >_B &= \delta(E-E')\delta(a,a'), \qquad \text{for } (E,E' < 0); \end{aligned} \tag{2.11}$$

$$\eta(-E)\,\eta(E')\; {}_B\!\!< H_o,A_o;E,a|H_o,A_o;E',a' > = 0 \tag{2.11a}$$

$$\eta(-E)\,\eta(E') < H_o,A_o;E,a|H_o,A_o,E',a' > = 0. \tag{2.11b}$$

We can define the projection operator $\eta(-H_o)$ by

$$\eta(-H_o) = \int\!\!\int |H_o,A_o;E,a > \eta(-E)dEda\; {}_B\!\!< H_o,A_o,E,a| \tag{2.12}$$

where the integration is carried out over the intervals ΔE_i. The extended space is defined by

$$\eta(H_o) + \eta(-H_o) = I. \tag{2.13}$$

The operator $\eta(-H_o)$ can be shown to be a projection operator which maps the Hilbert space into zero and the space added to the Hilbert space to form the full space into itself. A general vector $|\Phi >$ in the full space can be written as

$$(2.14)\qquad \langle q|\Phi\rangle = \iint \langle q|H_o,A_o;E,a\rangle\ \eta(E)dEda\ \langle H_o,A_o;E,a|\Phi\rangle$$

$$+\iint \langle q|H_o,A_o;E,a\rangle\,\eta(-E)dEda\ {}_B\langle H_o,A_o;E,a|\Phi\rangle,$$

where the first integral goes over the positive E axis and the second integral goes over the intervals ΔE_i.

In (2.14) the H_o representative of $|\Phi\rangle$ which is $\langle H_o,A_o;E,a|\Phi\rangle$ is a quadratically integrable function of E, a for E > 0. The function ${}_B\langle H_o,A_o;E,a|\emptyset\rangle$ is an integrable function of E, a in the intervals ΔE_i for E < 0. The definition of ${}_B\langle H_o,A_o;E,a|\Phi\rangle$ for E < 0 outside the intervals ΔE_i is immaterial.

Let us now consider some properties of the projection operators $\eta(H_o)$, $\eta(-H)$. First of all we note

$$(2.15)\qquad \eta(H_o)|H_o,A_o;E,a\rangle = \eta(E)|H_o,A_o;E,a\rangle$$

$$\eta(-H_o)|H_o,A_o;E,a\rangle = \eta(-E)|H_o,A_o;E,a\rangle.$$

The projection operator $\eta(-H_o)$ maps the Hilbert space into zero and maps that part of the vector space orthogonal to the Hilbert space into itself. By definition (2.12) and properties (2.7), (2.7a) and (2.7b)

$$(2.16)\qquad \eta(-H_o)\eta(H_o) = 0,\quad \eta^2(H_o) = \eta(H_o),\quad \eta^2(-H_o) = \eta(-H_o),$$

$$\eta(H_o)\eta(-H_o) = 0.$$

If T is any operator defined in the whole extended space then

$$T = T\eta(H_o) + T\eta(-H_o),$$

where $T\eta(H_o)$ is an operator which is zero when it operates on vectors orthogonal to the Hilbert space and where $T\eta(-H_o)$ is zero when it operates on the Hilbert space. All the operators defined in Part I may be considered to be of the form $T\eta(H_o)$ and hence most of the properties of the various operators discussed in

Part I will have analogues to operators of this character appearing here. The principal purpose of the present paper is to define operators over the full space, particularly the operators U, $U_{\pm}$, and W, i.e., to define $U\eta(-H_o)$, etc. It will not be necessary, however, to extend $L\eta(H_o)$, $M_{\pm}(H_o)$, as will be clear from the subsequent work.

The formal Hermitian adjoint of $T\eta(H_o)$ is $\eta(H_o)T^*$. If T commutes with H_o, it can be shown formally that

(2.17) $$\eta(H_o)T^* = T^*\eta(H_o).$$

Hence if such an operator operates on Hilbert space, its adjoint will still operate on the Hilbert space and maps vectors orthogonal to that space into zero. If R is another operator which commutes with H_o, one can show

(2.18) $$R\eta(H_o)T\eta(H_o) = RT\eta(H_o).$$

Hence products of such operators R and T acting on Hilbert space can be obtained by projecting on Hilbert space the product of the operators defined on the complete space. We shall use the properties (2.17) and (2.18) often without referring to them explicitly.

3. The eigenfunctions of the perturbed Hamiltonian and the transformation operator

A. The eigenfunctions of the continuous spectrum; the operators $U\eta(H_o)$, $U_{\pm}\eta(H_o)$, $W\eta(H_o) = W_c$

Let us consider the eigenfunctions $|H,A;E,a>$ of $H = H_o + \epsilon V$. As in Part I we introduce the operator U such that

(3.1) $$|H,A;E,a> = U|H_o,A_o;E,a>.$$

When $E > 0$ the eigenfunctions $|H_o,A_o;E,a>$ are those which span the Hilbert space.

But when $E = E_i$, where E_i is one of the point eigenvalues of H, we have

(3.2) $$|H,A;E_i,a> \; = \; U|H_o,A_o;E_i,a> ,$$

where $|H_o,A_o;E_i,a>$ is one of the vectors added to form the extended space. In fact these elements were added in order that (3.1) should hold for all values of E in the spectrum of H.

Let us consider the continuous spectrum of H. We shall obtain expressions for $U\eta(H_o)$ $U_\pm\eta(H_o)$, S, etc., analogous to those obtained in Part I where the continuous part of the spectrum which we are considering was the entire spectrum. The various expressions that are given below are obtained in an almost identical manner as those for the analogous operators of Part I. Therefore, instead of carrying out the derivations in detail, we shall indicate only the more important relationships.

For the case of the continous spectrum, (3.1) may be written

(3.2) $$\begin{aligned}|H,A;E,a> &= U\eta(E)|H_o,A_o;E,a> \\ &= U\eta(H_o)|H_o,A;E,a> \qquad (E > 0).\end{aligned}$$

In a manner similar to that used in Section 3 of Part I it can be shown that $U\eta(H_o)$ satisfies the equation

(3.3) $$U\eta(H_o) = L\eta(H_o) + \int \frac{P}{E-H_o} VU\eta(H_o)\delta(E-H_o)dE ,$$

where L is an arbitrary operator which commutes with H_o, and where as in Part I,

(3.3a) $$\delta(E-H_o) = \int |H_o,A_o;E,a> da < H_o,A_o;E,a| .$$

The integral in (3.3) is formally taken over the whole spectrum of the extended operator H_o. The factor $\eta(H_o)$ in the integral, however, in effect cuts out the negative part.

Now, as in Part I, there are two operators, $U_\pm\eta(H_o)$, which are particularly interesting and whose integral equations can be obtained by selecting $L\eta(H_o)$ pro-

perly. These operators are defined by the conditions

(3.4) $$\lim_{t \to -\infty} e^{iH_o t} e^{-iHt} U_- \eta(H_o)|\emptyset> = \eta(H_o)|\emptyset>,$$

(3.4a) $$\lim_{t \to +\infty} e^{iH_o t} e^{-iHt} U_+ \eta(H_o)|\emptyset> = \eta(H_o)|\emptyset>,$$

where $\eta(H_o)|\emptyset>$ is an arbitrary state in Hilbert space. As in Part I, $U_\pm \eta(H_o)$ satisfy

(3.5) $$U_\pm \eta(H_o) = \eta(H_o) + \varepsilon \int \gamma_\pm(E-H_o) V U_\pm \eta(H_o) \delta(E-H_o) dE.$$

The scattering operator S is defined by

(3.6) $$\lim_{t \to +\infty} e^{iH_o t} e^{-iHt} U_- \eta(H_o)|\emptyset> = S\eta(H_o)|\emptyset>,$$

where, as before, $\eta(H_o)|\emptyset>$ is an arbitrary state in Hilbert space. It can be shown that

(3.7) $$S = \eta(H_o) - 2\pi i\varepsilon \int \delta(E-H_o) V U_- \eta(H_o) \delta(E-H_o) dE$$

and that its inverse is given by

(3.8) $$S^{-1} = \eta(H_o) + 2\pi i\varepsilon \int \delta(E-H_o) V U_+ \eta(H_o) \delta(E-H_o) dE.$$

From (3.7) and (3.8) it is clear that S and S^{-1} can be written

(3.9) $$S = S\eta(H_o),$$

(3.10) $$S^{-1} = S^{-1}\eta(H_o)$$

and therefore that S and S^{-1} maps the space orthogonal to the Hilbert space into zero.

The general operator $U\eta(H_o)$ may be expressed in terms of $U_\pm \eta(H_o)$ as follows:

(3.11) $$U\eta(H_o) = U_\pm \eta(H_o) M_\pm \eta(H_o),$$

where

(3.12) $$M_{\pm}\eta(H_o) = L\eta(H_o) \mp i\epsilon\int\delta(E-H_o)VU\eta(H_o)\delta(E-H_o)dE.$$

From (3.12) it is clear that $M_{\pm}\eta(H_o)$ commutes with H_o. It can be shown that $M_{\pm}\eta(H_o)$ has an inverse in Hilbert space which commutes with H_o and which we shall denote by $M_{\pm}^{-1}\eta(H_o)$:

(3.13) $$M_{\pm}^{-1}\eta(H_o)M_{\pm}\eta(H_o) = M_{\pm}\eta(H_o)M_{\pm}^{-1}\eta(H_o) = \eta(H_o);$$

alternatively, noting that $M_{\pm}^{-1}$ commutes with H_o and using (2.13), we can write

(3.13a) $$M_{\pm}^{-1}M_{\pm}\eta(H_o) = M_{\pm}M_{\pm}^{-1}\eta(H_o) = \eta(H_o).$$

It can also be shown that

(3.14) $$\eta(H_o)U_{\pm}^{*}U_{\pm}\eta(H_o) = \eta(H_o),$$

which is a generalization of (4.21) of Part I. Equation (3.14) is essentially the normalization condition on the eigenfunctions

(3.14a) $$|H,A;E,a>_{\pm} = U_{\pm}\eta(H_o)|H_o,A_o;E,a>$$

(see Part I), namely

(3.14b) $$\eta(E)\eta(E')\,_{\pm}<H,A;E,a|H,A;E',a'>_{\pm} = \eta(E)\delta(E-E')\delta(a,a').$$

From (3.11) and (3.13) the corresponding relation for U is

(3.15) $$W_c\eta(H_o)U^{*}U\eta(H_o) = \eta(H_o)$$

where

(3.16) $$W_c\eta(H_o) = M_{\pm}^{-1}\eta(H_o)M_{\pm}^{-1*}\eta(H_o) = M_{\pm}^{-1}M_{\pm}^{*-1}\eta(H_o) = \eta(H_o)W_c.$$

It is to be noted that $W_c\eta(H_o)$ is a positive definite operator which has an inverse in Hilbert space. Equation (3.15) expresses the orthogonality relations between the eigenfunctions of the continuous spectrum of H associated

with the weight operator $W_c \eta(H_o)$.

Two expressions for S whose analogues appear in Part I are

$$S = \eta(H_o)\, U_+^* \, U_- \eta(H_o), \tag{3.17}$$

$$S = M_+ \eta(H_o) M_-^{-1} \eta(H_o) = M_+ M_-^{-1} \eta(H_o). \tag{3.18}$$

B. The eigenfunctions of the discrete spectrum; the operator $U\,\eta(-H_o)$

Let us now consider the eigenfunctions of the discrete spectrum of H, namely $|H,A;E_i,a>$. We should first note that the nature of the degeneracy operator A and its eigenvalues may be completely different for the discrete spectrum of H and for the continuous spectrum. In the case of the continuous spectrum the operator A may be chosen so that its eigenvalues are not countable (i.e., A may have a continuous spectrum). However, in the case of point eigenvalues E_i of H, the degeneracy is always countable, and in most applications is finite for a given value of E_i. Hence the operator A, when operating on that subspace of Hilbert space spanned by the eigenstates of the discrete spectrum of H, will have to be defined so as to have countable eigenvalues.

In order that the spectrum of the extended operator H_o have the same spectrum as H, it is necessary that the degeneracy operator A_o and its eigenvalues of additional eigenvectors $|H_o,A_o;E,a>$ which are introduced for values of E in the neighborhood ΔE_i of each eigenvalue E_i of H, have the same point spectrum as the eigenvalues of A in the eigenstate $|H,A;E_i,a>$.

We may then write, since $E_i < 0$,

$$\begin{aligned} |H,A;E_i,a> &= U\,|H_o,A_o;E_i,a> \\ &= U\,\eta(-E)\,|H_o,A_o;E_i,a> \\ &= U\,\eta(-H_o)\,|H_o,A_o;E_i,a>. \end{aligned} \tag{3.19}$$

For each value of a and E_i the operator maps an 'eigenvector' of the extended operator H_0 into an eigenvector H with the same value of a as a degeneracy label.

Generally the eigenfunctions of H corresponding to the discrete spectrum satisfy the following orthogonality relation:

$$< H,A;E_i,a|H,A;E_j,b > \; = \; \delta(i,j) < a|\omega_d^{-1}(E_i)|b >, \tag{3.20}$$

where $\delta(i,j)$ is the Kronecker δ. The matrix $< a|\omega_d^{-1}(E_i)|b >$ is a positive definite Hermitian matrix in the space of eigenfunctions of the operator A corresponding to a fixed eigenvalue E_i of H. In the case where the eigenfunctions belonging to the same eigenvalue E_i but having different degeneracy labels have been made orthogonal to each other, $< a|\omega_d^{-1}(E_i)|b >$ would have the form

$$< a|\omega_d^{-1}(E_i)|b > \; = \; C_{ia}\delta(a,b) \; ,$$

The constant C_{ia} (which is always positive) is the normalization constant for the eigenfunction $|H,A;E_i,a >$, that is,

$$< H,A;E_i,a|H,A;E_i,a > \; = \; C_{ia} \; .$$

The operator $< a|\omega_d^{-1}(E_i)|b >$ has a positive-definite inverse which we denote by $< a|\omega_d(E_i)|b >$; the latter, by definition, satisfies the relation

$$\begin{aligned} &\sum_b < a|\omega_d(E_i)|b > < b|\omega_d^{-1}(E_i)|b > \\ &= \sum_b < a|\omega_d^{-1}(E_i)|b > < b|\omega_d(E_i)|c > = \delta(a,c). \end{aligned} \tag{3.21}$$

There is one other orthogonality relation which we should note, namely the relation which expresses the orthogonality between the eigenfunctions of the discrete and continuous spectrum of H. It is

$$\eta(E)\,\eta(-E_i) < H,A;E,a|H,A;E_i,b > \; = \; 0. \tag{3.22}$$

C. The completeness theorem for H; definition of H in the extended space

The principal difference between the results of Parts I and II arises from the fact that in the present case the Hilbert space is spanned by the eigenfunctions belonging to the discrete as well as the continuous eigenfunctions of H.

Let us consider any state $\eta(H_o)|\emptyset>$ in Hilbert space. Further, let us take for the eigenfunctions of the continuous spectrum either the outgoing or incoming eigenstates $|H,A;E,a>_\pm = U_\pm \eta(H_o)|H_o,A_o;E,a>$. The arbitrary state $\eta(H_o)|\emptyset>$ can then be expanded in the following way:

$$\begin{aligned}\eta(H_o)|\emptyset> = &\iint |H,A;E,a>_\pm \eta(E)dEda \; {}_\pm< H,A;E,a|\eta(H_o)|\emptyset> \\ &+\sum_i\sum_{a,b} |H,A;E_i,a> < a|\omega_d(E_i)|b> < H,A;E_i,b|\eta(H_o)|\emptyset>.\end{aligned} \tag{3.23}$$

The coefficients of $|H,A;E,a>_\pm$ and $|H,A;E_i,a>$ in the expansion (3.23) follow from the normalization conditions (3.20) and (3.14b). Since $\eta(H_o)|\emptyset>$ is an arbitrary state in Hilbert space, (3.23) is equivalent to

$$\begin{aligned}&\iint |H,A;E,a>_\pm \eta(E)dEda \; {}_\pm< H,A;E,a|\eta(H_o) \\ &+\sum_i\sum_{a,b} |H,A;E_i,a> < a|\omega_d(E_i)|b> < H,A;F_i,b|\eta(H_o) = \eta(H_o).\end{aligned} \tag{3.24}$$

It is useful to define the positive definite matrices $< a|\omega_d(E)|b>$ in the previously described intervals ΔE_i so that for $E = E_i$ the operators $< a|\omega_d(E)|b>$ are the matrices $< a|\omega_d(E_i)|b>$ introduced earlier. On using (3.19), (3.14a) and (2.3) we have

$$\begin{aligned}&U_\pm \eta(H_o)U_\pm^* \eta(H_o) + \sum_i\sum_{a,b} U\eta(-H_o)\delta(E_i-H_o) \\ &\cdot\int |H_o,A_o;E,a> < a|\omega_d(E)|b> dE < H_o,A_o;E,b|\eta(-H_o)U^* \eta(H_o) = \eta(H_o),\end{aligned} \tag{3.25}$$

where the integral is taken over each of the intervals ΔE_i. Let us introduce

the operator

$$W_d\,\eta(-H_o) = \sum_{a,b}\int |H_o,A_o;E,a > < a|\omega_d(E)|b > dE < H_o,A_o;E,b|\,\eta(-H_o). \tag{3.26}$$

It is clear that $W_d\,\eta(-H_o)$ is a positive definite operator in the space orthogonal to the Hilbert space and that it commutes with H_o.

On using (3.11) and (3.16), Eq. (3.25) becomes

$$UWU^*\,\eta(H_o) = \eta(H_o), \tag{3.27}$$

where

$$W = W_c\,\eta(H_o) + \sum_i \delta(E_i-H_o)W_d\,\eta(-H_o). \tag{3.28}$$

Eq. (3.28) is the weight operator for the case where point eigenvalues exist. As can be seen, the weight operator is positive definite and has an inverse in the vector space. Eq. (3.28) provides a decomposition of W into two parts: W_c, which characterizes the orthogonality relations of the continuous spectrum of H (hence the subscript c for 'continuous'); and W_d, which characterizes the orthogonality relations of the discrete spectrum (hence the subscript d for 'discrete').

We have not yet discussed how H is to be defined in the extended space. The extension of H can be carried out by giving the vectors which span the extended space. Since we want the spectrum of the extended operator H to have the same spectrum as the spectrum of the extended operator H_o and hence of the original operator H, it is seen that the eigenstates of H which span the Hilbert space must also span the extended space. It is clear that the spectrum of H is thus preserved.

The effect of the extension of the definition of H is that equation (3.27) is replaced by

$$UWU^* = I. \tag{3.29}$$

4. More detailed discussion of the Q-representation and Q-extended operators

As in Part I we shall introduce the Q-representation and require that the operators K and K_o be triangular in terms of this representation, i.e.,

$$\text{(4.1)} \qquad \begin{aligned} < q|K|q' > &= 0, \qquad q' > q, \\ < q|K_o|q' > &= 0, \qquad q' > q, \end{aligned}$$

where K and K_o are given by

$$\text{(4.2)} \qquad \begin{aligned} U &= I + \varepsilon K, \\ U_o &= WU^* = I + \varepsilon K_o. \end{aligned}$$

Generally, the Q is defined only in the Hilbert space (i.e., only $Q\eta(H_o)$ is defined). Its eigenstates $|q>$ satisfy the completeness relation

$$\text{(4.3)} \qquad \int_{q_o}^{q_1} |q > dq < q| \eta(H_o) = \eta(H_o),$$

where q_1 and q_o are the upper and lower limits of the eigenvalues of Q. To extend the definition of Q into the whole vector space we write the completeness relation for the eigenfunctions $|q>$ as

$$\text{(4.4)} \qquad \int_{q_o}^{q_1} |q > dq < q| = I.$$

From (4.4) we have

$$\text{(4.5)} \qquad < q|q' > = \delta(q-q') = < q|I|q' >.$$

Eq. (4.4) means that any vector $|\emptyset >$ in the extended space has q-representative namely $< q|\emptyset >$. If the state $|\emptyset >$ is in Hilbert space it is quadratically integrable in the function $< q|\emptyset >$. If $\eta(-H_o)|\emptyset > \neq 0$, i.e., if $|\emptyset >$ has the component outside the Hilbert space, the functions $< q|\emptyset >$ are not quadratically integrable.

As usual, every operator A defined in the extended space can be given as an integral operator with the kernel $< q|A|q' >$, i.e., if $|\emptyset >$ is a state in the extended space $< q|A|\emptyset >$ can be written as (Using (4.4))

(4.6) $$< q|A|\emptyset > = \int_{q_0}^{q_1} < q|A|q' > dq' < q'|\emptyset >.$$

As in ordinary Hilbert space theory, the operator A is defined if the kernel $< q|A|q' >$ is given.

Let us consider now an operator of the form $A\,\eta(H_0)$. This operator operates in a non-trivial way only on the Hilbert space. It maps vectors orthogonal to the Hilbert space into zero. The kernel $< q|A\eta(H_0)|q' >$ is, of course, a known function of q and q'.

One might wish to extend the definition of the operator $A\eta(H_0)$ to an operator A which can be applied in a non-trivial way to the whole vector space and which equals $A\eta(H_0)$ when applied to the Hilbert space. One possible way of defining the extended operator A is to define the kernel $< q|A|q' >$ as a function of q and q' as being equal to the kernel $< q|A\eta(H_0)|q' >$.

(4.7) $$< q|A|q' > = < q|A\eta(H_0)|q' >.$$

It should be noted that Eq. (4.7) does <u>not</u> imply that $A = A\eta(H_0)$. An operator A obtained from $A\eta(H_0)$ by this means will be called a Q-extended operator. In Section 2 we took H_0 to be a Q-extended operator.

The simplest example of a Q-extended operator is the identity I, which is obtained from the operator $\eta(H_0)$ because we have

(4.8) $$< q|\eta(H_0)|q' > = \delta(q-q')$$

when $\eta(H_0)$ acts on the Hilbert space. Furthermore,

(4.9) $$< q|I|q' > = \delta(q-q') = < q|\eta(H_o)|q' >.$$

We shall require that the operator U be a Q-extended operator obtained from $U\eta(H_o)$. A consequence of this requirement is that

(4.10) $$< q|K|q' > = < q|K\eta(H_o)|q' >.$$

Since every operator can be written as an integral operator with a kernel, any operator which is given in terms of the Q-representation when acting on the Hilbert space has the same form as a Q-extended operator.

It should not be thought, however, that every operator acting on the full space is a Q-extended operator. For example, the weight operator W is not a Q-extended operator, since generally

$$< q|W\eta(H_o)|q' > = < q|W_c\eta(H_o)|q' >$$

does <u>not</u> equal

$$< q|W|q' > = < q|W_c\eta(H_o)|q' > + < q|W_d\eta(-H_o)|q' >.$$

5. Theorems on the inverse problem. The equation for K, K_o

We shall now present theorems analogous to those of Part I. We shall not go through the proofs because the proofs of Part I are essentially the same if the Hilbert space is extended properly.

> <u>Theorem I</u>. Let there be given a vector space spanned by the eigenfunctions of the extended operators H_o, A_o as described above, the negative point eigenvalues of H, E_i and the degeneracy of these eigenvalues being given. Further, let us prescribe the positive definite operator
>
> $$W = W_c\eta(H_o) + \sum_i \delta(E_i-H_o)W_d\,\eta(-H_o)$$
>
> in the vector space; W commutes with H_o and has an inverse. Then if the equations

$$(5.1) \qquad U_o = WU^*$$

$$(5.2) \qquad U_o = U^{-1}$$

can be solved for U, U_o, the operator H given by

$$(5.3) \qquad H = UH_oU_o$$

is a Hermitian operator whose eigenstates corresponding to the continuous spectrum are

$$(5.4) \qquad |H,A;E,a> = U\eta(E)|H_o,A_o;E,a> \qquad \text{for } 0 \leq E < 0$$

and whose eigenstates corresponding to the point eigenvalues E_i with the prescribed degeneracies are

$$(5.5) \qquad |H,A;E_i,a> = U|H_o,A_o;E_i,a>.$$

The eigenstates of H will satisfy the completeness relation

$$(5.6) \qquad \iiint |H,A;E,a> da < a|\omega_c(E)|b> \eta(E)dEdb < H,A;E,b| + \sum_i \sum_{a,b} |H,A;E_i,a> < a|\omega_d(E_i)|b> < H,A;E_i,b| = I,$$

where

$$< a|\omega_c(E)|b> \eta(E)$$

and

$$< a|\omega_d(E)|b> \eta(-E)$$

are defined by

$$(5.7) \quad < H_o,A_o;E,a|W_c\eta(H_o)|H_o,A_o;E',b> = \delta(E-E') < a|\omega_c(E)|b> \eta(E),$$

$$(5.8) \quad < H_o,A_o;E,a|W_d\eta(-H_o)|H_o,A_o;E',b> = \delta(E-E') < a|\omega_d(E)|b> \eta(-E).$$

Furthermore, the eigenfunctions will satisfy the normalization conditions

$$(5.9) \qquad \int < a|\omega_c(E)|b> db < H,A;E,b|H,A;F,c> = \delta(E-F)\delta(a,c),$$

$$(5.10) \qquad < H,A;E,b|H,A;E_i,c> = 0, \qquad (E > 0),$$

$$(5.11) \qquad \sum_b < a|\omega_d(E_i)|b> < H,A;E_i,b|H,A;E_j,c> = \delta(i,j)\delta(a,c).$$

The condition that W be a positive definite operator which commutes with H_o and which has an inverse is equivalent to requiring the same properties of $W_c \eta(H_o)$ and $W_d \eta(-H_o)$ in the Hilbert space and the vector space orthogonal to the Hilbert space respectively.

Theorem II. If we write $U = I + \varepsilon K$, $U_o = I + \varepsilon K_o$ and require K, K_o to be triangular in the Q-representation then $U_o = WU^*$ has a unique solution for U, U_o if W satisfies conditions analogous to those required in Part I.

Theorem III. It can be shown that if the extension of the Hilbert space is carried out properly then $U_o = U^{-1}$.

We shall now write the generalized Gelfand-Levitan equation for K. From (5.1) we have

$$UW = U_o^* . \tag{5.12}$$

Let us write

$$\begin{aligned} U &= I + \varepsilon K \\ U_o &= I + \varepsilon K_o \\ W &= \eta(H_o) + \varepsilon \Omega . \end{aligned} \tag{5.13}$$

Then (5.12) becomes

$$\eta(H_o) + \varepsilon \Omega + \varepsilon K \eta(H_o) + \varepsilon^2 K \Omega = I + \varepsilon K_o^* \tag{5.14}$$

or in terms of the Q-representation

$$\begin{aligned} &< q|\eta(H_o)|q' > + \varepsilon < q|\Omega|q' > + \varepsilon < q|K\eta(H_o)|q' > \\ &\qquad + \varepsilon^2 < q|K\Omega|q' > = \delta(q-q') + \varepsilon < q|K_o^*|q' > . \end{aligned} \tag{5.15}$$

Now

$$< q|\eta(H_o)|q' > = \delta(q-q') \tag{5.16}$$

when $\eta(H_o)$ acts on Hilbert space; otherwise

$$< q|\eta(H_o)|q' > = 0.$$

Hence

(5.17) $$< q|\eta(H_o)|q' > \; = \; 0 \qquad (q > q').$$

From the triangularity condition (4.1) on K_o

(5.18) $$< q|K_o^*|q' > \; = \; 0 \qquad (q > q').$$

We now use the fact that K is a Q-extended operator and write

(5.19) $$< q|K\eta(H_o)|q' > \; = \; < q|K|q' >.$$

Hence, finally we obtain our equation for K, namely

(5.20) $$< q|K|q' > \; = - < q|\Omega|q' > - \; \varepsilon \int_{q_o}^{q} < q|K|q''> dq'' < q''|\Omega|q' >, \qquad (q > q'),$$

which is the same equation for $< q|K|q' >$ as obtained in Part I.

6. Conditions on the eigenfunctions $|H_o,A_o;E_i,a >$

The condition that $|H,A;E_i,a >$ be in Hilbert space and hence that the q-representative $< q|H,A;E_i,a >$ be a quadratically integrable function of q leads to a condition on $< q|H_o,A_o;E_i,a >$ if we assume K is triangular in the Q-representation. We can write

(6.1) $$< q|H,A;E_i,a > \; = \; < q|H_o,A_o;F,a > + \; \varepsilon \int_{q_o}^{q} < q|K|q' > dq' < q'|H_o,A_o;E_i,a >.$$

Now since the second term approaches zero as q approaches q_o, we see that the quadratic integrability of $< q|H,A;E,a >$ implies that $< q|H_o,A_o;E_i,a >$ be a quadratically integrable function of q in the neighborhood of $q = q_o$.

It appears, in fact, that a sufficient condition on the extension of the Hilbert space to guarantee the validity of the three theorems of Section 5 is the condition that $< q|H_o,A_o;E_i,a >$ satisfy

$$(6.2) \qquad \int_{q_o}^{q_a} < H_o,A_o;E_i,a|q' > dq' < q'|H_o,A_o;E_i,a > \quad < \infty \quad \text{for } q_a < q_1 .$$

That is, the added eigenfunctions $< q|H_o,A_o;E_i,a >$ are 'essentially' in Hilbert space if one replaces these functions by zero in the vicinity of $q = q_1$. The functions $< q|H_o,A_o;E_i,a >$ will have to be singular at $q = q_1$ in order that these eigenfunctions span a space bigger than Hilbert space. Then the q-representative $< q|\emptyset >$ of any state $|\emptyset >$ as a function of q is quadratically integrable:

$$(6.3) \qquad \int_{q_o}^{q_a} < \emptyset|q > dq < q|\emptyset > \quad < \infty \quad \text{for } q_a < q_1 .$$

Those states $|\emptyset >$ which are in Hilbert space are, of course, quadratically integrable in $q_o \leq q \leq q_1$ be definition:

$$(6.4) \qquad \int_{q_o}^{q_1} < \emptyset|q > dq < q|\emptyset > \quad < \infty.$$

States which are not in Hilbert space will have representatives $< q|\emptyset >$ which have singularities for $q = q_1$ which are so severe that the square $< q|\emptyset >$ does not exist:

$$(6.5) \qquad \int_{q_o}^{q_1} < \emptyset|q > dq < q|\emptyset > \; = \; \infty.$$

Under the conditions of the extension of the Hilbert space, one can say that the Hilbert space is 'dense' in the vector space; that is, every state in the vector space $< q|\emptyset >$ can be considered as being approximated by an element of Hilbert space for $q < q_1$.

The vector space of Ref. [2] has essentially this property.

References

[1]. I. Kay and H. E. Moses, The determination of the scattering potential from the spectral measure function; CX-18, Institute of Mathematical Sciences, Division of Electromagnetic Research, New York University.

[2] I. Kay, On the determination of a linear system from the reflection coefficient; EM-74, Institute of Mathematical Sciences, Division of Electromagnetic Research, New York University.

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